

## CAS/STN FILE 'HCAPLUS' ENTERED AT 15:57:47 ON 06 JUN 2005

L1 1 S US2004106007/PN  
 L2 SEL PLU=ON L1 1- RN : 42 TERMS  
 L3 6414 S L2  
 L4 1 S L1 AND L3

## FILE 'STNGUIDE' ENTERED AT 15:58:07 ON 06 JUN 2005

## FILE 'REGISTRY' ENTERED AT 15:58:41 ON 06 JUN 2005

L5 STRUCTURE UPLOADED  
 L6 5 SEA SSS SAM L5  
 L7 STRUCTURE UPLOADED  
 L8 50 SEA SSS SAM L7  
 L9 67 SEA SSS FUL L5  
 L10 165429 SEA SSS FUL L7  
 L11 0 S L9 AND L10  
 L12 0 S L9 AND IR/ELS  
 L13 8127 S L10 AND IR/ELS  
 L14 40519 S CL/ELS AND L10  
 L15 8 S CL/ELS AND L9  
 L16 2974 S L13 AND L14  
 L17 2974 S L16 AND P/ELS  
 L18 651 S L17 AND F/ELS  
 L19 7584 S (L9 OR L10) AND IRIDIUM  
 L20 64546 S (L9 OR L10) AND PHOSPHO?  
 L21 32053 S (L9 OR L10) AND CHLORO?  
 L22 88 S L19 AND L20 AND L21  
 L23 26 S L22 AND F/ELS

## FILE 'HCAPLUS' ENTERED AT 16:05:00 ON 06 JUN 2005

L24 36 S (L22 OR L23)  
 L25 35 S L24 AND IRIDIUM  
 L26 30 S L24 AND IR  
 L27 16 S L24 AND PHOSPHO?

## FILE 'REGISTRY' ENTERED AT 16:05:42 ON 06 JUN 2005

L28 15526 S (L8 OR L9 OR L10 OR L11 OR L12 OR L13 OR  
 L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR  
 L23) AND 5/NR  
 L29 16490 S (L8 OR L9 OR L10 OR L11 OR L12 OR L13 OR  
 L14 OR L15 OR L16 OR L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR  
 L23) AND 7/NR  
 L30 13621 S L29 AND TRIPHEN?  
 L31 12872 S L28 AND TRIPHEN?  
 L32 3017 S (L30 OR L31) AND F/ELS  
 L33 587 S L32 AND CHLORO?  
 L34 50 S L32 AND CHLORIDE  
 L35 138 S (L33 OR L34) AND IRIDIUM  
 L36 4 S (L33 OR L34) AND PHOSPHORUS

## FILE 'HCAPLUS' ENTERED AT 16:07:59 ON 06 JUN 2005

L37 11 S L36  
 L38 75 S L35  
 L39 24 S L9  
 L40 0 S L38 AND L39  
 L41 0 S L37 AND L39  
 L42 0 S L38 AND L39  
 L43 23 S (L37 OR L38 OR L39) AND 2002-2005/PY, PRY  
 L44 29 S (L37 OR L38 OR L39) AND 1993-2001/PY, PRY  
 L45 87 S (L37 OR L38 OR L39) NOT L43  
 L46 99 S L44 OR L45  
 L47 110 S (L37 OR L38 OR L39)  
 L48 3 S L46 AND BIDENT?  
 L49 0 S L46 AND DENTATE?  
 L50 40 S L46 AND LIGAND?  
 L51 35 S L37 OR L39  
 L52 14 S L51 NOT L43  
 L53 31 S L44 OR L52  
 L54 63 S L37 OR L44 OR L48 OR L50 OR L52 OR L53  
 L55 37 S L54 AND (F OR F3 OR CF3 OR TRIFLUOR? OR  
 FLUOR#####)

## FILE 'REGISTRY' ENTERED AT 16:35:31 ON 06 JUN 2005

L57 78293 S L10 AND N/ELS  
 L58 10539 S L57 AND F/ELS  
 L59 19939 S L57 AND CL/ELS  
 L60 3380 S L57 AND IR/ELS  
 L61 77441 S L57 AND PHOSPH?  
 L62 1776 S L58 AND L59  
 L63 293 S L60 AND L62  
 L64 289 S L61 AND L63  
 L65 288 S L64 AND IRIDIUM  
 L66 96 S L65 AND TRIFLUOR?  
 L67 0 S PHOSPHOIRID?  
 L68 314 S CHLOROIRID?  
 L69 8214 S IRID? (2A) (CHLORO OR CHLORIDE)  
 L70 5061 S IRID? (2A) PHOSPH#####  
 L71 0 S L66 AND L68  
 L72 64 S L66 AND L69  
 L73 19 S L66 AND L70  
 L74 16 S L72 AND L73

## FILE 'HCAPLUS' ENTERED AT 16:40:06 ON 06 JUN 2005

L75 4 S L74

## FILE 'REGISTRY' ENTERED AT 16:41:30 ON 06 JUN 2005

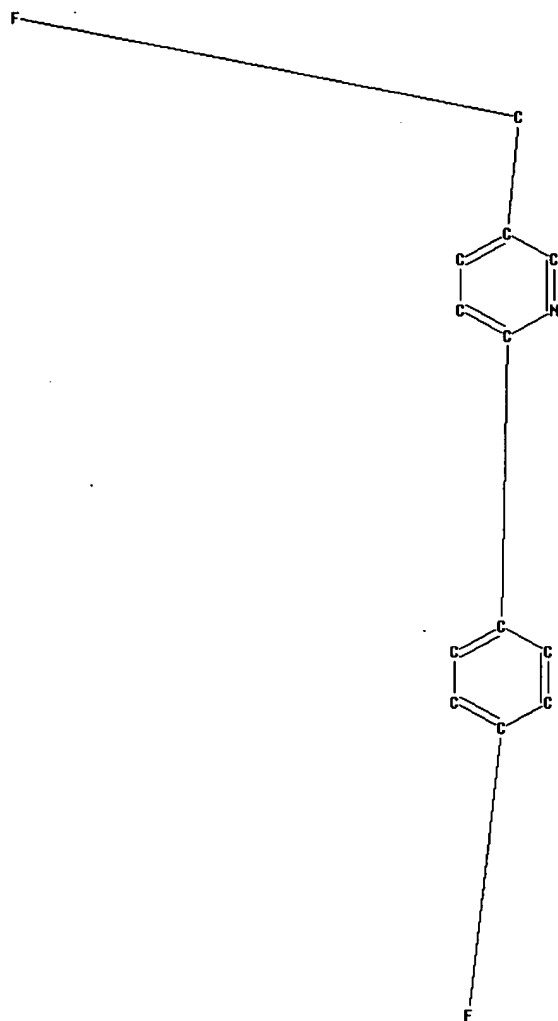
L76 67711 S TRIPHENYL? AND (L57 OR L58 OR L59 OR L60  
 OR L61 OR L62 OR L63 OR L64 OR L65 OR L66 OR L67 OR L68 OR L69  
 OR L70 OR L71 OR L72 OR L73 OR L74 OR L75)  
 L77 2257 S L76 AND TRIFLUOR?  
 L78 301 S L77 AND N/ELS AND CL/ELS  
 L79 298 S L78 AND P/ELS  
 L80 96 S L79 AND IR/ELS

## FILE 'HCAPLUS' ENTERED AT 16:42:17 ON 06 JUN 2005

L81 29 S L80  
 L82 20 S L81 NOT (L75 OR L55)

6/6/05

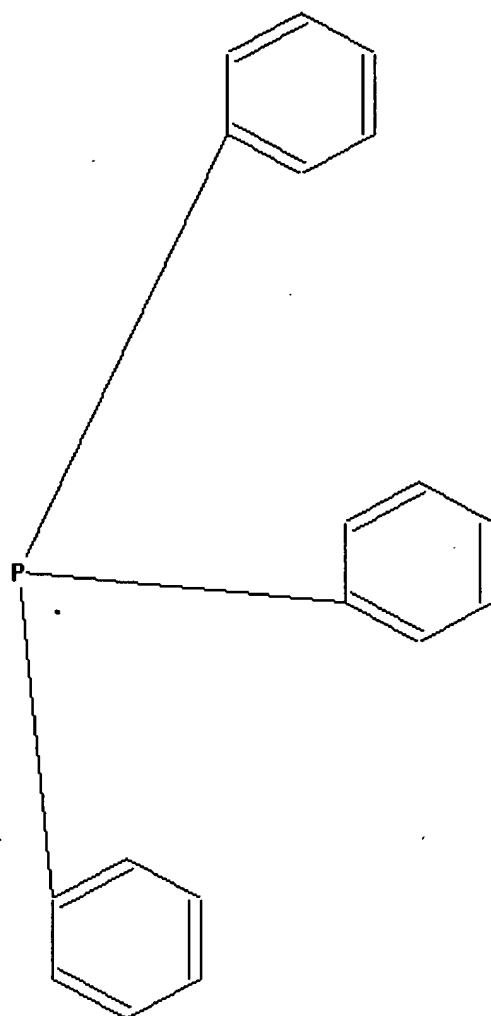
Structure in Set L5



6/6/05

10/696,095

Structure in Set L7



(FILE 'CAS REGISTRY FILE ' ENTERED AT 08:40:29 ON 07 JUN 2005)

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L1      STRUCTURE UPLOADED
L2      2 SEA SSS SAM L1
L3      13335 S S1
L4      510 S L3 AND PYRIDIN?
L5      185 S L3 AND (IRIDIUM OR IR/ELS)
L6      2498 S L3 AND CL/ELS
L7      5869 S L3 AND N/ELS
L8      1 S L5 AND L4
L9      59 S L5 AND L6
L10     35 S L5 AND L7
L11     170 S L4 AND L6
L12     0 S L4 AND L5 AND L7 AND L6
L13     1 S L4 AND L5 AND L7
L14     0 S L4 AND L5 AND L6
L15     170 S L4 AND L7 AND L6
L16     0 S L5 AND L15
L17     0 S L13 NOT L8
L18     1169 S L3 AND (FLUOR? OR F/ELS)
L19     228 S L3 AND (TRIFLUOROMETH?)
L20     140 S (L4 OR L5 OR L6 OR L7 OR L8 OR L9 OR L10
OR L11 OR L12 OR L13 OR L14 OR L15) AND L19
L21     266881 S PHENYLTRIS OR TRIPHENYL OR TRI PHENYL OR
TRIS PHENYL OR TRISPHENYL
L22     471 S L3 AND L21
L23     334 S (L4 OR L5 OR L6 OR L7 OR L8 OR L9 OR L10
OR L11 OR L12 OR L13 OR L14 OR L15 OR L16 OR L17 OR L18 OR L19
OR L20) AND L22
L24     188 S L23 AND 1/NC
L25     269 S L23 AND PHOSPHIN?
L26     2 S L23 AND CHLOR##### (4A) IRIIDIUM
D FIDE 1-2
L27     82 S L23 AND F/ELS
L28     20 S TRIFLUOROMETH? AND L27
D FIDE 1-28
L29     0 S L27 AND IR/ELS
L30     18 S L22 AND IR/ELS
L31     1 S 148353-70-2/RN

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FILE 'HCAPLUS' ENTERED AT 09:00:36 ON 07 JUN 2005

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L32     2 S L31
L33     SEL PLU=ON L32 1- RN :      53 TERMS

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FILE 'CAS REGISTRY FILE ' ENTERED AT 09:01:32 ON 07 JUN 2005

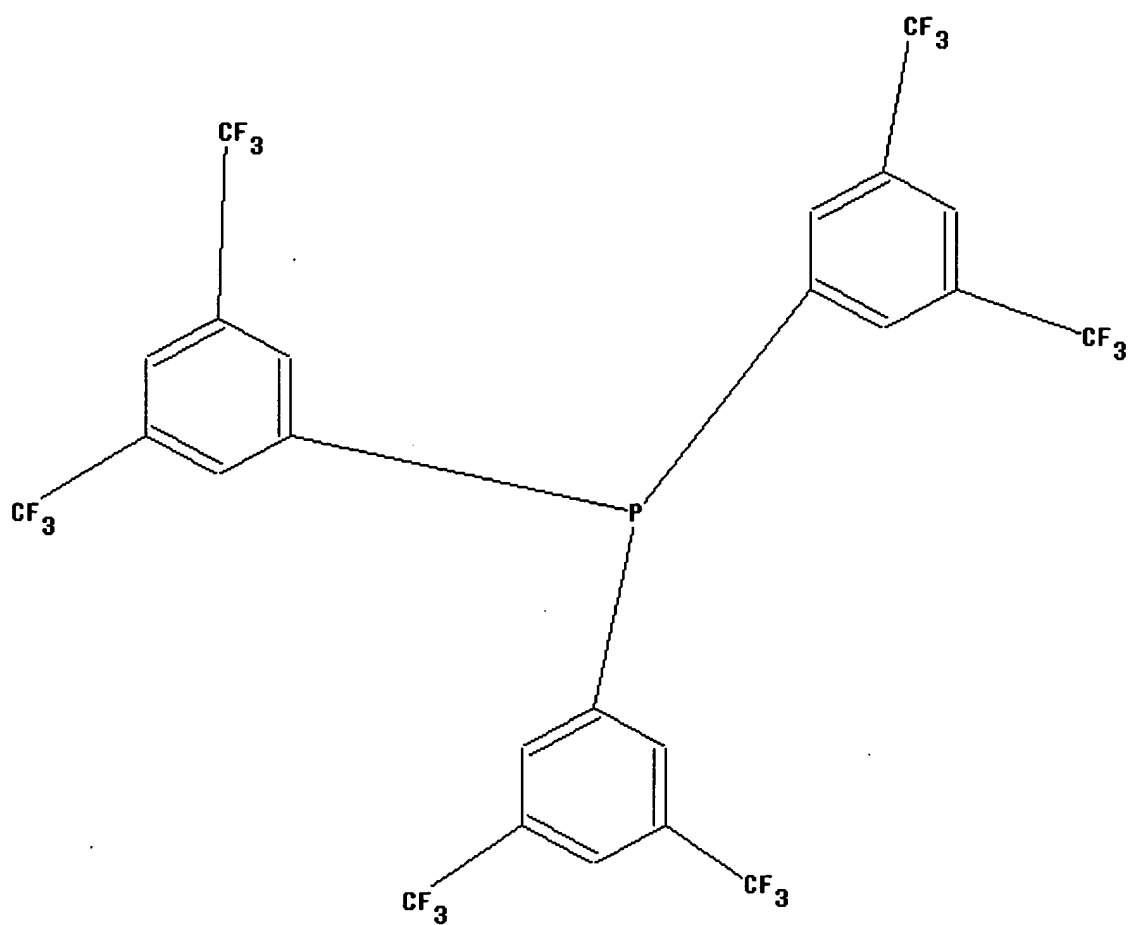
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L34     53 S L33
L35     26 S L34 AND IR/ELS
L36     3311 S L33/CRN
L37     2 S L36 AND P/ELS AND IR/ELS
L38     25 S L35 AND P/ELS
L39     25 S L38 AND (CL OR N)/ELS
L40     13 S L39 AND (TRI OR TRIS)
L41     25 S L39 AND (BI OR DI OR BIS)
L42     13 S L40 AND L41
L43     13 S L42 NOT L37

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6/7/05

## Structure in Set L1



L45 ANSWER 1 OF 1 HCAPLUS COPYRIGHT ACS on STN

AN 2001:839278 HCAPLUS

DN 136:95098

ED Entered STN: 19 Nov 2001

TI Substituent effects on aurophilicity and .pi.-.pi. interaction in crystals of arylphosphine-Au(I) derivatives. Synthesis and x-ray structural studies of compounds (CX<sub>3</sub>C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>P-Au-X and {(CF<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>}<sub>3</sub>P-Au-X

AU Nunokawa, Keiko; Onaka, Satoru; Tatematsu, Tsutomu; Ito, Mitsuhiro; Sakai, Jyun

CS Department of Environmental Technology, Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, 466-8555, Japan

SO Inorganica Chimica Acta (2001), 322(1,2), 56-64

CODEN: ICHAA3; ISSN: 0020-1693

PB Elsevier Science S.A.

LA English

OS CASREACT 136:95098

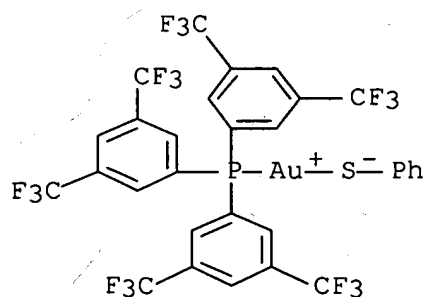
AB Substituent effects on aurophilic interactions were explored by single-crystal x-ray diffraction methods for Au(I) complexes of monodentate phosphines, R'<sub>3</sub>P-Au-X (X = Cl, Sph, and Spy). When a CF<sub>3</sub> substituent is introduced at a meta position of the Ph ring in Ph<sub>3</sub>P, aurophilicity was accrued in ClAuP(m-CF<sub>3</sub>C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>. However, aurophilicity was weakened by introducing two CF<sub>3</sub> groups at both meta positions. When a CF<sub>3</sub> substituent is substituted for a H atom in the para position or when a CH<sub>3</sub> substituent is introduced in the meta and/or para positions, such an effect was not obsd. for R'<sub>3</sub>PAuCl and R'<sub>3</sub>PAuSph. Most dimers constructed by aurophilicity appear to be reinforced by .pi.-.pi. interactions between the Ph ring of the Sph ligand or the pyridine ring of the Spy ligand and one of the Ph rings in the R'<sub>3</sub>P ligand. A novel ladder-like supra mol. architecture is created in the crystal of {3,5-(F<sub>3</sub>C)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>}<sub>3</sub>PAuSph, and a tetramer is formed in the crystal of Ph<sub>3</sub>PAuSpy by aurophilic and .pi.-.pi. interactions. Substituent effects on important bond lengths are discussed.

IT 385815-88-3P

(dimeric through weak Au-Au interaction; prepn. and crystal and mol. structure in study of substituent effects on aurophilic and .pi.-.pi. interactions)

RN 385815-88-3 HCAPLUS

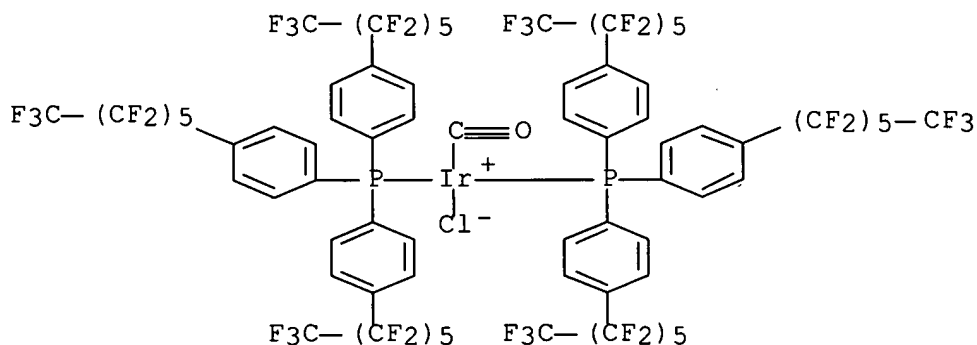
CN Gold, (benzenethiolato)[tris[3,5-bis(trifluoromethyl)phenyl]phosphine-.kappa.P]- (9CI) (CA INDEX NAME)



L43 ANSWER 1 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN  
 RN 219938-12-2 CAS REGISTRY FILE  
 ED Entered STN: 24 Feb 1999  
 CN Iridium, carbonylchlorobis[tris[4-(tridecafluorohexyl)phenyl]phosphine- $\kappa$ P]-, (SP-4-3)- (9CI) (CA INDEX NAME)  
 MF C73 H24 Cl F78 Ir O P2  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS, USPAT2, USPATFULL  
 DT.CA CAPLUS document type: Journal; Patent  
 RL.P Roles from patents: USES (Uses)  
 RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	IC6	16	IC6	46.150.18	16



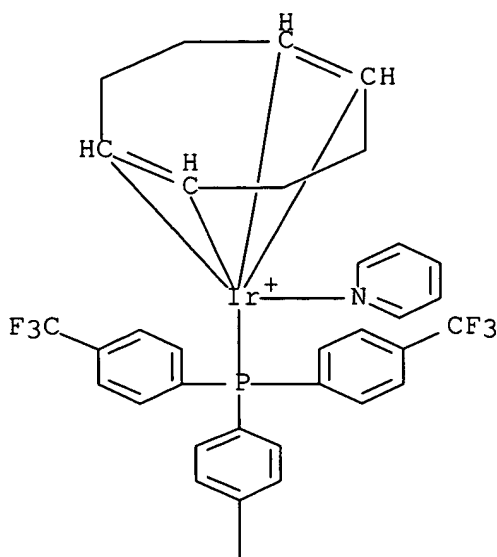
2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)



L106 ANSWER 3 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN  
 RN 186494-78-0 CAS REGISTRY FILE  
 ED Entered STN: 27 Feb 1997  
 CN Iridium(1+), [(1,2,5,6-.eta.)-1,5-cyclooctadiene] (pyridine) [tris[4-(trifluoromethyl)phenyl]phosphine-.kappa.P]-, hexafluorophosphate(1-)  
 (9CI) (CA INDEX NAME)  
 MF C34 H29 F9 Ir N P . F6 P  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); USES (Uses)

CM 1  
 CRN 186494-77-9  
 CMF C34 H29 F9 Ir N P  
 CCI CCS

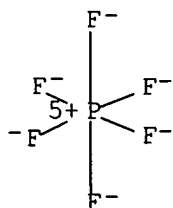
PAGE 1-A



PAGE 2-A



CM 2  
 CRN 16919-18-9  
 CMF F6 P  
 CCI CCS



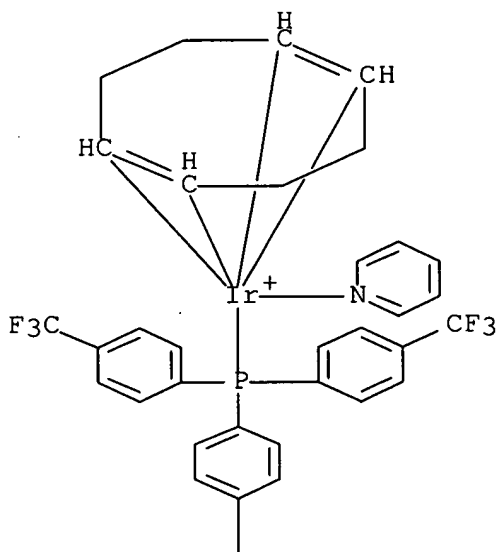
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L106 ANSWER 4 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN  
 RN 186494-77-9 CAS REGISTRY FILE  
 ED Entered STN: 27 Feb 1997  
 CN Iridium(1+), [(1,2,5,6-eta.)-1,5-cyclooctadiene] (pyridine) [tris[4-(trifluoromethyl)phenyl]phosphine-kappa.P]- (9CI) (CA INDEX NAME)  
 MF C34 H29 F9 Ir N P  
 CI CCS, COM  
 SR CA

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	3
C5N	NC5	6	C5N	46.156.30	1
C2Ir-C2Ir-	IrC2-IrC2-	3-3-5-5	C8Ir	280.7.3	1
C4Ir-C4Ir	IrC4-IrC4				

PAGE 1-A



PAGE 2-A

CF<sub>3</sub>

L106 ANSWER 10 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN

RN 173950-46-4 CAS REGISTRY FILE

ED Entered STN: 07 Mar 1996

CN Iridium(1+), carbonyl(.eta.5-2,4-cyclopentadien-1-yl)hydro[tris[4-(trifluoromethyl)phenyl]phosphine]- (9CI) (CA INDEX NAME)

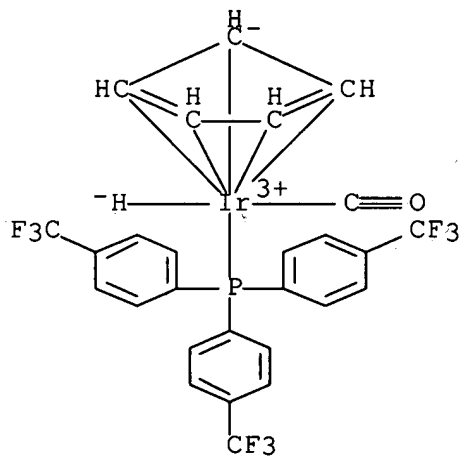
MF C27 H18 F9 Ir O P

CI CCS, COM

SR CA

## Ring System Data

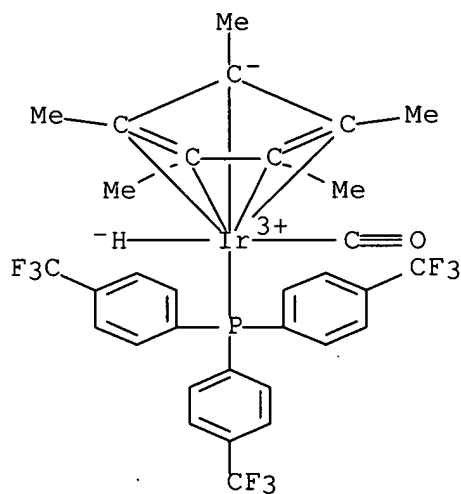
Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C2Ir-C2Ir-	IrC2-IrC2-	3-3-3-3-3	C5Ir	23.15.1	1
C2Ir-C2Ir-	IrC2-IrC2-				
C2Ir	IrC2				
C6	C6	6	C6	46.150.18	3



L106 ANSWER 8 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN  
 RN 173950-58-8 CAS REGISTRY FILE  
 ED Entered STN: 07 Mar 1996  
 CN Iridium(1+), carbonylhydro[(1,2,3,4,5-eta.)-1,2,3,4,5-pentamethyl-  
 2,4-cyclopentadien-1-yl][tris[4-(trifluoromethyl)phenyl]phosphine]-  
 (9CI) (CA INDEX NAME)  
 MF C32 H28 F9 Ir O P  
 CI CCS, COM  
 SR CA

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C2Ir-C2Ir-	IrC2-IrC2-	3-3-3-3-3	C5Ir	23.15.1	1
C2Ir-C2Ir-	IrC2-IrC2-				
C2Ir	IrC2				
C6	C6	6	C6	46.150.18	3

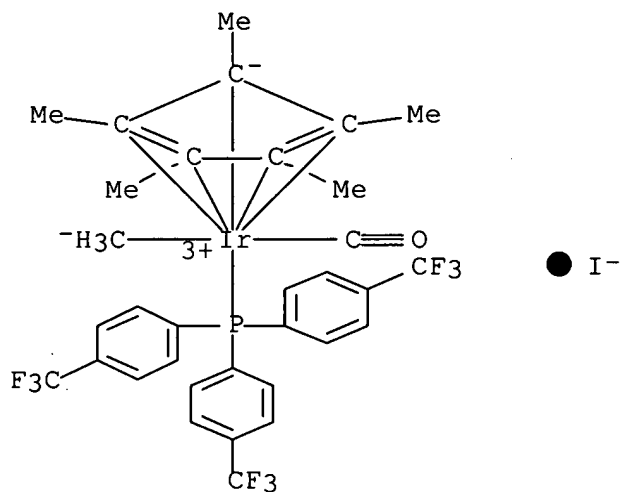


L106 ANSWER 5 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN

RN 173950-78-2 CAS REGISTRY FILE  
 ED Entered STN: 07 Mar 1996  
 CN Iridium(1+), carbonylmethyl[(1,2,3,4,5-eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl][tris[4-(trifluoromethyl)phenyl]phosphine]-, iodide (9CI) (CA INDEX NAME)  
 MF C33 H30 F9 Ir O P . I  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA CAPLUS document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation)  
 CRN (740064-45-3)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C2Ir-C2Ir-	IrC2-IrC2-	3-3-3-3-3	C5Ir	23.15.1	1
C2Ir-C2Ir-	IrC2-IrC2-				
C2Ir	IrC2				
C6	C6	6	C6	46.150.18	3

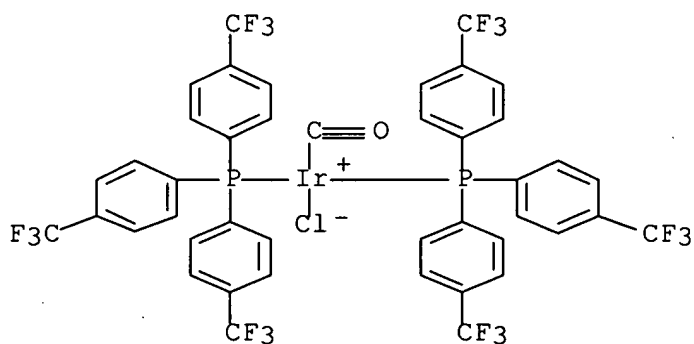


1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L43 ANSWER 4 OF 13 CAS REGISTRY FILE COPYRIGHT ACS on STN  
 RN 148353-70-2 CAS REGISTRY FILE  
 ED Entered STN: 29 Jun 1993  
 CN Iridium, carbonylchlorobis[tris[4-(trifluoromethyl)phenyl]phosphine-  
 .kappa.P]-, (SP-4-3)- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Iridium, carbonylchlorobis[tris[4-(trifluoromethyl)phenyl]phosphine]-  
 , (SP-4-3)-  
 MF C43 H24 Cl F18 Ir O P2  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS  
 DT.CA Caplus document type: Journal  
 RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP  
 (Properties); RACT (Reactant or reagent)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	IC6	16	IC6	46.150.18	6



2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

----- 6/7/05

10/696,095

REGISTRY COPYRIGHT 2005 ACS on STN

RN 603-35-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Phosphine, triphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN EPCAT-P

CN JC 263

CN NSC 10

CN NSC 215203

CN P 100

CN P 100 (accelerator)

CN PP 360

CN TPP

CN Triphenylphosphane

CN Triphenylphosphide

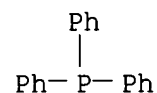
CN **Triphenylphosphine**

CN Triphenylphosphorus

FS 3D CONCORD

DR 112771-47-8

MF C18 H15 P



See HELP PROPERTIES for information about property data sources in REGISTRY.

18641 REFERENCES IN FILE CA (1907 TO DATE)

2656 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

18668 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L55 ANSWER 8 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 2001:581384 HCAPLUS

DN 135:349716

ED Entered STN: 10 Aug 2001

TI New, efficient electroluminescent materials based on organometallic Ir complexes

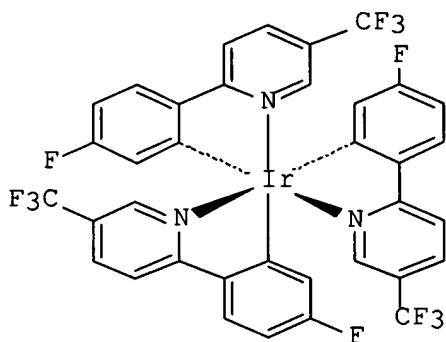
AU Grushin, Vladimir V.; Herron, Norman; LeCloux, Daniel D.; Marshall, William J.; Petrov, Viacheslav A.; Wang, Ying

CS Central Research and Development, Experiment Station, E. I. DuPont de Nemours and Co., Inc., Wilmington, DE, 19880-0328, USA

SO Chemical Communications (Cambridge, United Kingdom) (2001), (16), 1494-1495

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry



I

AB Reaction of aq.  $\text{IrCl}_3$  with **fluorinated** 2-arylpiperidines in the presence of  $\text{AgO}_2\text{CCF}_3$  afforded fifteen fac-tris-cyclometalated arylpyridine Ir complexes (e.g., I) exhibiting excellent processing and electroluminescent properties which can be fine-tuned via systematic control of the nature and position of the substituents on the arom. rings. Single-crystal x-ray structures were obtained for I and three other analogous cyclometalated arylpyridine Ir complexes. Nearly all the arylpyridine Ir complexes exhibited fully reversible redn. and oxidn. waves.

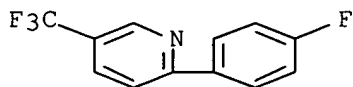
IT 370878-58-3, 5-(Trifluoromethyl)-2-(4-fluorophenyl)pyridine

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclometalation with aq. iridium chloride)

RN 370878-58-3 HCAPLUS

CN Pyridine, 2-(4-fluorophenyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

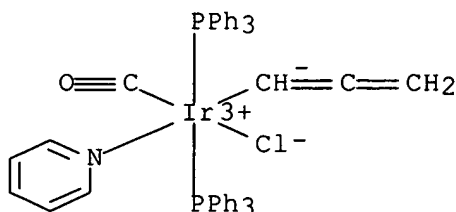




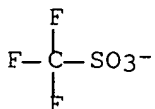
L55 ANSWER 16 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 1997:175133 HCAPLUS  
 DN 127:95391  
 ED Entered STN: 15 Mar 1997  
 TI Coordination of Aniline to an (.eta.1-Allenyl)iridium Complex Leading to Hydroanilination  
 AU Chen, Jwu-Ting; Chen, Yu-Kun; Chu, Jiane-Bond; Lee, Gene-Hsiang; Wang, Yu  
 CS Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan  
 SO Organometallics (1997), 16(7), 1476-1483  
 CODEN: ORGND7; ISSN: 0276-7333  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 29-13 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 75  
 OS CASREACT 127:95391  
 AB Formation of the N-arylated .eta.3-aza-TMM complexes of iridium from regioselective hydroanilination of an octahedral (.eta.1-allenyl)iridium complex has been studied. (OC-6-42)-Ir(Cl)(PPh<sub>3</sub>)<sub>2</sub>(OTf)(CO)(.eta.1-CHCCH<sub>2</sub>)(2) undergoes the substitution of L (L = NH<sub>3</sub>, NH<sub>2</sub>NH<sub>2</sub>, MeNH<sub>2</sub>, EtNH<sub>2</sub>, iPrNH<sub>2</sub>, PhCH<sub>2</sub>NH<sub>2</sub>) for the triflate **ligand** to yield {(OC-6-42)-Ir(Cl)(PPh<sub>3</sub>)<sub>2</sub>(L)(CO)(.eta.1-CHCCH<sub>2</sub>)}(OTf) (3d-i). In contrast, the reactions of 2 with XC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> (X = F, NO<sub>2</sub>, MeO, H, Me), Ph<sub>2</sub>NH, and Ph(Me)NH result in regioselective addn. at the allenyl **ligand**, thereby generating the N-arylated .eta.3-aza-TMM complexes 5a-g. The mechanistic studies confirm that the hydroanilination is preceded by the formation of an aniline-ligated intermediate. The crystal structure of (OC-6-42)-Ir(Cl)(PPh<sub>3</sub>)<sub>2</sub>(NHSO<sub>2</sub>Ph)(CO)(.eta.1-CHCCH<sub>2</sub>), {Ir(Cl)(PPh<sub>3</sub>)<sub>2</sub>(CO)[.eta.3-CH<sub>2</sub>C(NPh<sub>2</sub>)CH<sub>2</sub>]}(OTf) (5f), and {Ir(Cl)(PPh<sub>3</sub>)<sub>2</sub>(CO)[.eta.3-CH<sub>2</sub>C(NPhMe)CH<sub>2</sub>]}(OTf) (5g) were detd.  
 IT 191852-00-3P 191852-03-6P 191852-22-9P  
 191852-26-3P 191852-29-6P 191852-32-1P 191852-51-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 191852-03-6 HCAPLUS  
 CN Iridium(1+), carbonylchloro-1,2-propadienyl(pyridine)bis(triphenylphosphine)-, (OC-6-42)-, salt with trifluoromethanesulfonic acid (1:1)

CM 1  
 CRN 191852-02-5  
 CMF C45 H38 Cl Ir N O P2  
 CCI CCS

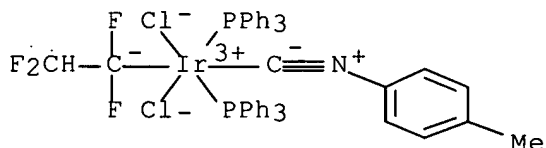


CM 2  
 CRN 37181-39-8  
 CMF C F3 O3 S

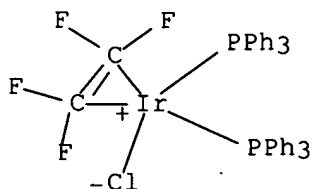


L55 ANSWER 20 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 1995:232547 HCAPLUS  
 DN 122:187760  
 ED Entered STN: 08 Dec 1994  
 TI Tetrafluoroethyl complexes of iridium(III) derived from a tetrafluoroethylene complex of iridium(I). A study of .alpha.-fluoride abstraction and determination of the structure of  $\text{IrCl}_2(\text{CF}_2\text{CF}_2\text{Cl})(\text{CO})(\text{PPh}_3)_2$   
 AU Burrell, Anthony K.; Clark, George R.; Rickard, Clifton E. F.; Roper, Warren R.  
 CS Department of Chemistry, University of Auckland, Private Bag 92019, Auckland, N. Z.  
 SO Journal of Organometallic Chemistry (1994), 482(1-2), 261-9  
 CODEN: JORCAI; ISSN: 0022-328X  
 PB Elsevier  
 DT Journal  
 LA English  
 CC 29-13 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 75  
 OS CASREACT 122:187760  
 AB Treatment of the tetrafluoroethylene complex,  $\text{IrCl}(\eta^2\text{-C}_2\text{F}_4)(\text{PPh}_3)_2$ , (1), with HCl or  $\text{Cl}_2$  gives  $\text{IrCl}_2(\text{CF}_2\text{CF}_2\text{H})(\text{PPh}_3)_2$  (2) or  $\text{IrCl}_2(\text{CF}_2\text{CF}_2\text{Cl})(\text{PPh}_3)_2$  (3), resp. These coordinately unsatd. complexes react with various neutral ligands to give stable, six-coordinate, tetrafluoroethyl and halotetrafluoroethyl complexes. The single crystal x-ray structure of one of these compds., the carbonyl deriv. of 3,  $\text{IrCl}_2(\text{CF}_2\text{CF}_2\text{Cl})(\text{CO})(\text{PPh}_3)_2$  was detd. The acetonitrile deriv. of 2,  $\text{IrCl}_2(\text{CF}_2\text{CF}_2\text{H})(\text{CH}_3\text{CN})(\text{PPh}_3)_2$  undergoes a reaction with HCl that proceeds through the intermediate fluorocarbene complex,  $[\text{IrCl}_2(\text{:CFCF}_2\text{H})(\text{CH}_3\text{CN})(\text{PPh}_3)]^+$ , to give, upon hydrolysis,  $\text{IrCl}_2(\text{C}[\text{O}]\text{CF}_2\text{H})(\text{CH}_3\text{CN})(\text{PPh}_3)_2$  (19). The acetonitrile ligand, by virtue of its position trans to the acyl group, can be thermally displaced from 19 to give  $\text{IrCl}_2(\text{C}[\text{O}]\text{CF}_2\text{H})(\text{PPh}_3)_2$  (20). The vacant coordination site in 20 can be filled by other neutral ligands. Thermal treatment of any of the acyl complexes results finally in a reverse migration process and formation of  $\text{IrCl}_2(\text{CF}_2\text{H})(\text{CO})(\text{PPh}_3)_2$ .  
 IT 161566-63-8P 161566-69-4P 161566-73-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 161566-63-8 HCAPLUS  
 CN Iridium, dichloro(1-isocyano-4-methylbenzene)(1,1,2,2-tetrafluoroethyl)bis(triphenylphosphine)-, (OC-6-12)-

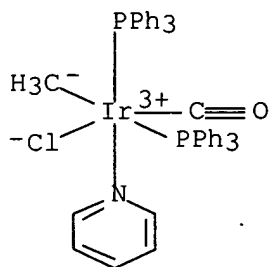


IT 27709-91-7  
 (prepn. of tetrafluoroethyl complexes of iridium derived from tetrafluoroethylene complex of iridium and study of fluoride abstraction)  
 RN 27709-91-7 HCAPLUS  
 CN Iridium, chloro(.eta.2-tetrafluoroethene)bis(triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)

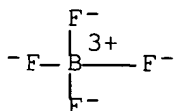


L55 ANSWER 23 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 1982:465469 HCAPLUS  
 DN 97:65469  
 ED Entered STN: 12 May 1984  
 TI Organometallic Lewis acids; metal complexes with weakly coordinated ligands. IX. Hydrido- and methyliridium(III) complexes with weakly coordinated anionic ligands; route to cationic iridium(III) complexes  
 AU Olgemöeller, Bernhard; Bauer, Herbert; Loebermann, Hartmut; Nagel, Ulrich; Beck, Wolfgang  
 CS Inst. Anorg. Chem., Univ. Muenchen, Munich, Fed. Rep. Ger.  
 SO Chemische Berichte (1982), 115(6), 2271-86  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DT Journal  
 LA German  
 CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 29, 75  
 AB The oxidative addn. of HX (X = O<sub>3</sub>SCF<sub>3</sub>, O<sub>3</sub>SC<sub>4</sub>F<sub>9</sub>, BF<sub>4</sub>) and Me<sub>3</sub>O[BF<sub>4</sub>] to trans-Ir(CO)Cl(PPh<sub>3</sub>)<sub>2</sub> gave via cis or trans addn. Ir(CO)Cl(PPh<sub>3</sub>)<sub>2</sub>HX (I) and Ir(CO)Cl(PPh<sub>3</sub>)<sub>2</sub>(BF<sub>4</sub>)Me (II), resp. I and II react with weak neutral .sigma.- or .pi.-donors to give Ir(CO)Cl(PPh<sub>3</sub>)<sub>2</sub>HL (L = MeCN, PPh<sub>3</sub>, H<sub>2</sub>O, Me<sub>2</sub>CO, THF) or [Ir(CO)Cl(PPh<sub>3</sub>)<sub>2</sub>Me(py)]BF<sub>4</sub>, resp. I (X = BF<sub>4</sub>), in which H and X are in axial positions and the 2 PPh<sub>3</sub> groups are trans, is triclinic, space group P.hivin.1, with a 1002.0(2), b 1080.5(6), c 2060.1(7) pm, .alpha. 74.80(3).degree., .beta. 77.58(2).degree., .gamma. 65.36(3).degree., d. (x-ray) = 1.63, d. (exptl.) = 1.63(1), Z = 2. I, II, and the cationic Ir(III) complexes were characterized by IR and NMR spectra.  
 IT 82474-50-8P 82510-05-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 82474-50-8 HCAPLUS  
 CN Iridium(1+), carbonylchloromethyl(pyridine)bis(triphenylphosphine)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 82474-49-5  
 CMF C43 H38 Cl Ir N O P2  
 CCI CCS

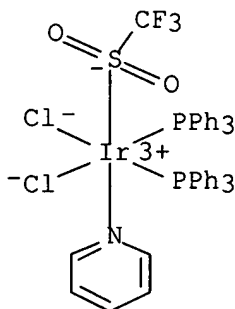


CM 2  
 CRN 14874-70-5  
 CMF B F4  
 CCI CCS



L55 ANSWER 27 OF 37 HCAPLUS COPYRIGHT ACS on STN

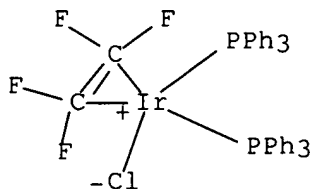
AN 1977:494748 HCAPLUS  
 DN 87:94748  
 ED Entered STN: 12 May 1984  
 TI Preparation and characterization of five and six-coordinated iridium(III) complexes containing S-, O- or O,O'-trifluoromethanesulfinato groups  
 AU Blake, Daniel M.; Chung, Y. L.  
 CS Dep. Chem., Univ. Texas, Arlington, TX, USA  
 SO Journal of Organometallic Chemistry (1977), 134(3), 327-34  
 CODEN: JORCAI; ISSN: 0022-328X  
 DT Journal  
 LA English  
 CC 78-7 (Inorganic Chemicals and Reactions)  
 AB The oxidative addn. of trifluoromethanesulfonyl chloride to trans-[IrX(CO)(PPh<sub>3</sub>)<sub>2</sub>] yields as the only product an Ir(III) complex, [IrXCl(OS(O)CF<sub>3</sub>)(CO)(PPh<sub>3</sub>)<sub>2</sub>] (X = Cl, Br) in which the O-sulfinato group is trans to the carbonyl ligand. This is in contrast to the behavior of hydrocarbon sulfonyl halides which give exclusively S-bonded forms with the sulfinato group trans to chloride. The S- and O,O'-trifluoromethanesulfinato isomers of the compd. [IrCl<sub>2</sub>(O<sub>2</sub>SCF<sub>3</sub>)(PPh<sub>3</sub>)<sub>2</sub>] were prepd. and characterized. Addn. of CO or pyridine to either of these isomers gives [IrCl<sub>2</sub>(S(O)O<sub>2</sub>CF<sub>3</sub>)(PPh<sub>3</sub>)<sub>2</sub>L] (L = CO or C<sub>5</sub>H<sub>5</sub>N) in which the added Lewis base is trans to an S-sulfinato group.  
 IT 63771-67-5P 63816-41-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 63771-67-5 HCAPLUS  
 CN Iridium, dichloro(pyridine)[(trifluoromethyl)sulfonyl]bis(triphenylphosphine)-, (OC-6-14)- (9CI) (CA INDEX NAME)



L55 ANSWER 30 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 1974:146275 HCAPLUS  
 DN 80:146275  
 ED Entered STN: 12 May 1984  
 TI Tetrafluoroethylene complexes of iridium(I)  
 AU Van Gaal, H. L. M.; Van der Ent, A.  
 CS Unilever Res., Vlaardingen, Neth.  
 SO Inorganica Chimica Acta (1973), 7(4), 653-9  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 CC 29-13 (Organometallic and Organometalloidal Compounds)  
 AB The chlorobis(ethylene)iridium(I) dimer,  $[\text{IrCl}(\text{C}_2\text{H}_4)_2]_2$  and acetylacetonatobis(ethylene)iridium(I),  $\text{Ir}(\text{acac})(\text{C}_2\text{H}_4)_2$ , react with  $\text{C}_2\text{F}_4$  to give mixed ethylenetetrafluoroethylene complexes, in which the ethylene ligand may be replaced by alkenes such as cyclooctene and 1,5-cyclooctadiene. A no. of neutral ligands can be added to these complexes with or without alkene substitution. In several complexes a strong ir-absorption in the region 1350-1500  $\text{cm}^{-1}$  is attributed to (C:C)-stretching of the fluoroalkene. PMR expts. with  $\text{Ir}(\text{acac})(\text{C}_2\text{H}_4)_2$  and  $\text{Ir}(\text{acac})(\text{C}_2\text{H}_4)(\text{C}_2\text{F}_4)$  indicated that the rate of associative ethylene exchange and the barrier to rotation around the metal-ethylene bond were related to the basicity of the metal substrate. Alkene addn. is discussed in terms of nucleophilic attack of the metal on the empty antibonding alkene-orbitals.

IT 27709-91-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 27709-91-7 HCAPLUS  
 CN Iridium, chloro(.eta.2-tetrafluoroethene)bis(triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)



L75 ANSWER 3 OF 4 HCAPLUS COPYRIGHT ACS on STN

AN 1986:626938 HCAPLUS

DN 105:226938

ED Entered STN: 26 Dec 1986

TI Trifluoromethyl and mixed hydrido trifluoromethyl complexes of iridium(III) as potential precursors of an iridium(I) trifluoromethyl complex

AU Greene, T. R.; Roper, W. R.

CS Dep. Chem., Univ. Auckland, Auckland, N. Z.

SO Journal of Organometallic Chemistry (1986), 299(2), 245-50

CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

OS CASREACT 105:226938

AB Abstraction of iodide from  $\text{Ir}(\text{CF}_3)\text{ClI}(\text{CO})(\text{PPh}_3)_2$  by  $\text{AgSbF}_6$  in the presence of acetonitrile yields the cationic complex  $[\text{Ir}(\text{CF}_3)\text{Cl}(\text{MeCN})(\text{CO})(\text{PPh}_3)_2]^+ [\text{SbF}_6]^-$  (I). The acetonitrile group of I is readily displaced, and I reacts with p-tolyl isocyanide to yield  $[\text{Ir}(\text{CF}_3)\text{Cl}(\text{CNC}_6\text{H}_4\text{Me}-4)(\text{CO})(\text{PPh}_3)_2]^+ [\text{SbF}_6]^-$  (II). The addn. of NaOMe to II results in the methoxy ester complex  $\text{Ir}(\text{CF}_3)(\text{COOMe})\text{Cl}(\text{CNC}_6\text{HMe}-4)(\text{PPh}_3)_2$ . The acetonitrile ligand of I is also displaced by anions, including  $\text{H}^-$ . Thus I reacts with  $\text{LiEt}_3\text{BH}$  to give  $\text{Ir}(\text{CF}_3)\text{HCl}(\text{CO})(\text{PPh}_3)_2$  (III), in which the hydrido and trifluoromethyl ligands are mutually trans. In contrast, the addn. of excess  $\text{NaBH}_4$  to I affords the novel dihydrido complex  $\text{trans-IR}(\text{CF}_3)\text{H}_2(\text{CO})(\text{PPh}_3)_2$  (IV). Investigations into the potential use of III and IV as precursors of an Ir(I) complex such as  $\text{Ir}(\text{CF}_3)(\text{CO})(\text{PPh}_3)_2$  are also described.

IT 105250-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction with sodium methoxide)

RN 105250-41-7 HCAPLUS

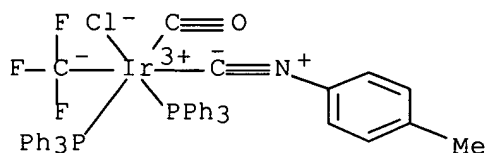
CN Iridium(1+), carbonylchloro(1-isocyano-4-methylbenzene)(trifluoromethyl)bis(triphenylphosphine)-, (OC-6-42)-, (OC-6-11)-hexafluoroantimonate(1-)  
(9CI) (CA INDEX NAME)

CM 1

CRN 105250-40-6

CMF C46 H37 Cl F3 Ir N O P2

CCI CCS

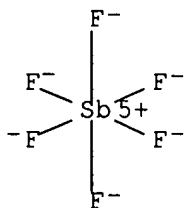


CM 2

CRN 17111-95-4

CMF F6 Sb

CCI CCS



L55 ANSWER 1 OF 37 HCAPLUS COPYRIGHT ACS on STN

AN 2003:590870 DN 139:159040 ED Entered STN: 01 Aug 2003.

TI Photoactive lanthanide complexes with phosphine oxides, phosphine oxide-sulfides, pyridine N-oxides, and **phosphine** oxide-pyridine N-oxides, and thin film OLED devices made with such complexes

IN Grushin, Vladimir; Herron, Norman; Petrov, Viacheslav Alexandrovich; Radu, Nora Sabina; Wang, Ying

PA E. I. Du Pont De Nemours and Company, USA

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003144487	A1	20030731	US 2002-185484	20020627 <--
	US 6875523	B2	20050405		
	CA 2449740	AA	20031106	CA 2002-2449740	20020703 <--
	WO 2003091688	A2	20031106	WO 2002-US21024	20020703 <--
	WO 2003091688	A3	20040805		
	EP 1465595	A2	20041013	EP 2002-807315	20020703 <--
	TW 593626	B	20040621	TW 2002-91114969	20020705 <--
	US 2005095202	A1	20050505	US 2004-11676	20041214 <--
	US 2005095203	A1	20050505	US 2004-11699	20041214 <--
	US 2005095204	A1	20050505	US 2004-11700	20041214 <--
	US 2005100511	A1	20050512	US 2004-11668	20041214 <--
	US 2005106109	A1	20050519	US 2004-11074	20041214 <--
PRAI	US 2001-303283P	P	20010705	<--	
	US 2002-185484	A3	20020627		
	WO 2002-US21024	W	20020703		

OS MARPAT 139:159040

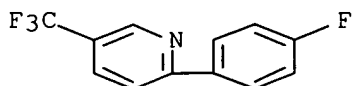
AB The present invention is generally directed to luminescent lanthanide compds. with phosphine oxide, phosphine oxide-sulfide, pyridine N-oxide, and phosphine oxide-pyridine N-oxide **ligands**, esp. with .beta.-enolate co-**ligands**. It also relates to thin film OLED electronic devices in which the active layer includes the photoactive lanthanide complex. Thus, Tb(PMBP)3(F5tpO)2 [PMBP = 4-isobutyryl-3-methyl-1-phenyl-5-pyrazolate, F5tpO = tris(pentafluorophenyl)phosphine oxide] was prepd. and its electroluminescent properties were measured along with 7 other prepd. complexes. Thin layer OLED devices were prepd. including a hole transport layer, electroluminescent layer comprising the lanthanide complexes of the invention, and at least one electron transport layer. Various hole and electron transport materials are also claimed. Cyclometalated iridium complexes derived from (un)substituted 2-phenylpyridines are preferred.

IT 370878-58-3P

(for prepn. of cyclometalated iridium complexes contg. pyridylphenyl ligand)

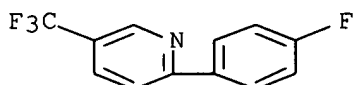
RN 370878-58-3 HCAPLUS

CN Pyridine, 2-(4-fluorophenyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



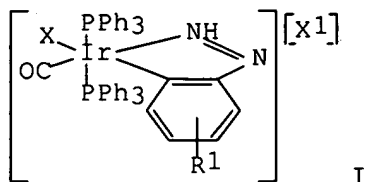
L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT ACS on STN  
 AN 2002:964786 DN 138:47038 ED Entered STN: 20 Dec 2002  
 TI Electroluminescent iridium compounds with fluorinated phenylpyridines,  
 phenylpyrimidines, and phenylquinolines and devices made with such compounds  
 IN Grushin, Vladimir; Lecloux, Daniel D.; Petrov, Viacheslav. A.; Wang, Ying  
 PA E. I. Du Pont de Nemours & Co., USA

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002190250	A1	20021219	US 2001-27421	20011220
US 6670645	B2	20031230		
US 2002121638	A1	20020905	US 2001-879014	20010612
EP 1424382	A2	20040602	EP 2004-4541	20010627
EP 1431288	A2	20040623	EP 2004-4542	20010627
EP 1431289	A2	20040623	EP 2004-4543	20010627
CA 2455844	AA	20030731	CA 2001-2455844	20011226
WO 2003063555	A1	20030731	WO 2001-US49522	20011226
CN 1520702	A	20040811	CN 2001-823216	20011226
EP 1466506	A1	20041013	EP 2001-991428	20011226
JP 2005516040	T2	20050602	JP 2003-563272	20011226
US 2004089867	A1	20040513	US 2003-696349	20031029
US 2004106007	A1	20040603	US 2003-696095	20031029 <--
US 2004108507	A1	20040610	US 2003-696003	20031029
US 2004188673	A1	20040930	US 2003-696060	20031029
US 2004191959	A1	20040930	US 2003-696401	20031029
US 2004094769	A1	20040520	US 2003-699411	20031030
US 2004075096	A1	20040422	US 2003-720967	20031124
US 2004116696	A1	20040617	US 2003-720954	20031124
US 2005095457	A1	20050505	US 2004-983119	20041105
<b>PRAI US 2000-215362P</b>	<b>P</b>	<b>20000630</b>		
US 2000-224273P	P	20000810		
US 2001-879014	A2	20010612		
EP 2001-950576	A3	20010627		
US 2001-27421	A3	20011220		
WO 2001-US49522	W	20011226		
US 2003-366295	A3	20030213		
OS MARPAT 138:47038				
AB Ir(III) compds. with substituted 2-phenylpyridines, phenylpyrimidines, and phenylquinolines, and devices, esp. electroluminescent devices, that are made with the Ir(III) compds., are described. Precursor ligands for the devices are also described.				
IT (iridium compds. with fluorinated phenylpyridines and phenylpyrimidines and phenylquinolines and electroluminescent devices based on the compds. and their precursors)				
RN 370878-58-3 HCAPLUS				
CN Pyridine, 2-(4-fluorophenyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)				





L75 ANSWER 4 OF 4 HCAPLUS COPYRIGHT ACS on STN  
 AN 1977:468478 HCAPLUS  
 DN 87:68478  
 ED Entered STN: 12 May 1984  
 TI Aryldiazonato- and aryldiazene complexes. Some orthometalated compounds derived from reactions of diazonium ions with carbonylchlorobis(triphenylphosphine)iridium  
 AU Gilchrist, Alan B.; Sutton, Derek  
 CS Dep. Chem., Simon Fraser Univ., Burnaby, BC, Can.  
 SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1977), (7), 677-82  
 CODEN: JCDTBI; ISSN: 0300-9246



AB A wide range of substituted aryldiazonium ions  $RN_2^+$  react with  $Ir(CO)Cl(PPh_3)_2$  and its F, Br, I, and  $OCIO_3$  analogs in benzene-EtOH or benzene-Me<sub>2</sub>CHOH to give orthometalated aryldiazene Ir(III) complexes I ( $X = F, Cl, Br, I, OCIO_3$ ;  $R_1 = H, F, Br, Cl, Me, CF_3, NH_2, NO_2, OMe$ ;  $X_1 = BF_4, ClO_4$ ). I may be deprotonated to give the corresponding orthometalated aryldiazonato complexes, and hydrogenated by  $H_2$  at 1 atm and 25.degree. in the presence of a Pd catalyst to give the corresponding orthometalated arylhydrazine complexes.

IT 63686-17-9P

(prepn., deprotonation, and hydrogenation reactions of)

RN 63686-17-9 HCAPLUS

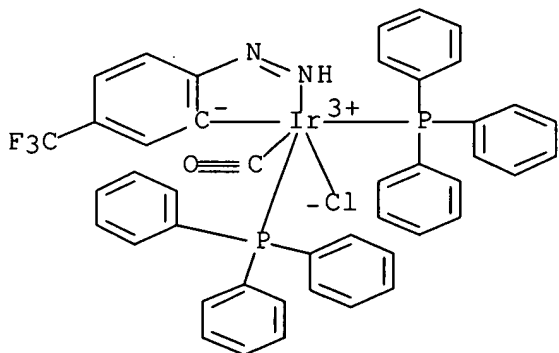
CN Iridium(1+), carbonylchloro[2-diazenyl-5-(trifluoromethyl)phenyl]bis(triphenylphosphine)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 63686-16-8

CMF C44 H34 Cl F3 Ir N2 O P2

CCI CCS



CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

